Preprint
UCRL-JC-141597

Thermal Decomposition of Trinitrotoluene (TNT) with a New One-Dimensional Time to Explosion (ODTX) Apparatus

T. D. Tran, R. L. Simpson, J. Maienschein, C. Tarver

This article was submitted to
32nd International Annual Conference of Institute of Chemistry Technology, Karlsruhe, Germany, July 3-6, 2001

March 23, 2001

U.S. Department of Energy

Lawrence Livermore National Laboratory

This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

THERMAL DECOMPOSITION OF TRINITROTOLUENE (TNT) WITH A NEW ONE-DIMENSIONAL TIME TO EXPLOSION (ODTX) APPARATUS

T. D. Tran, L. R. Simpson, J. Maienschein and C. Tarver

Energetic Materials Center

Lawrence Livermore National Laboratory

P. O. Box 808, Livermore, CA 94551

ABSTRACT

The thermal explosion of trinitrotoluene (TNT) is used as a basis for evaluating the performance of a new One-Dimensional-Time-to-Explosion (ODTX) apparatus. The ODTX experiment involves holding a 12.7 mm-diameter spherical explosive sample under confinement (150 MPa) at a constant elevated temperature until the confining pressure is exceeded by the evolution of gases during chemical decomposition. The resulting time to explosion as a function of temperature provides valuable decomposition kinetic information. A comparative analysis of the measurements obtained from the new unit and an older system is presented. Discussion on selected performance aspects of the new unit will also be presented.

The thermal explosion of TNT is highly dependent on the material. Analysis of the time to explosion is complicated by historical and experimental factors such as material variability, sample preparation, temperature measurement and system errors. Many of these factors will be addressed. Finally, a kinetic model using a coupled thermal and heat transport code (chemical TOPAZ) was used to match the experimental data.

INTRODUCTION

The thermal explosions of a wide variety of high explosives (HE) have been investigated using the One-Dimensional-Time-to-Explosion (ODTX) apparatus at Lawrence Livermore National Laboratory. Such experiments involved holding at constant elevated temperature a small spherical (12.7 mm-diameter) HE sample in two identical aluminum anvils that are confined at 150 MPa. The time to explosion is the elapsed time between the sample insertion (and anvil closure) and the rupture of containment. The time to explosion as a function of the temperature provides useful kinetic information on the material decomposition. The system was first reported in 1976 by Catalano et al. (1). The thermal decomposition of trinitrotoluene (TNT) was one of the first reactions studied in this

original work. Multi-step chemical kinetic decomposition modeling of TNT was first reported by Tarver et al. (2) and McGuire and Tarver (3).

We have recently built a new apparatus as a replacement. It incorporates new components, modern equipment and expanded diagnostic capabilities. Basic experimental design parameters such as sample size, anvil materials and dimension remain unchanged to facilitate comparison with previous work. The upgrades and new features include in-situ temperature sensing and control, faster sample loading, external (hydraulic) pressure sensor, and computer-controlled operation and data collection as well as provisions for additional diagnostics. The new system was designed to provide very accurate determination of the temperature and the time to explosion. A high level of accuracy in time to explosion is needed to investigate effects of factors such as sample heterogeneity, impurity, and confinement pressure on the decomposition kinetics. Such a study is now possible using the new ODTX unit.

The thermal decomposition of trinitrotoluene (TNT) was used to verify the performance of the new ODTX apparatus. It was chosen because of available historical ODTX data, its common use and its useful physical properties. TNT, for example, has a low melting point (~ 80°C). Since explosive thermal reactions occur at significantly higher temperatures (> 170°C), the behavior of a liquid explosive can eliminate complexities in kinetics derived from heterogeneity associated with porosity and particle size in pressed plastic bonded materials such as HMX-based composites. We expected that the molten TNT reaction would provide a higher resolution of any difference in the explosion times and temperature measurements inherent in the two systems. A comparative analysis of the measurements obtained from both the new and existing apparatuses is presented. This serves as a basis for reconciling the existing database with results from the new apparatus.

EXPERIMENTAL

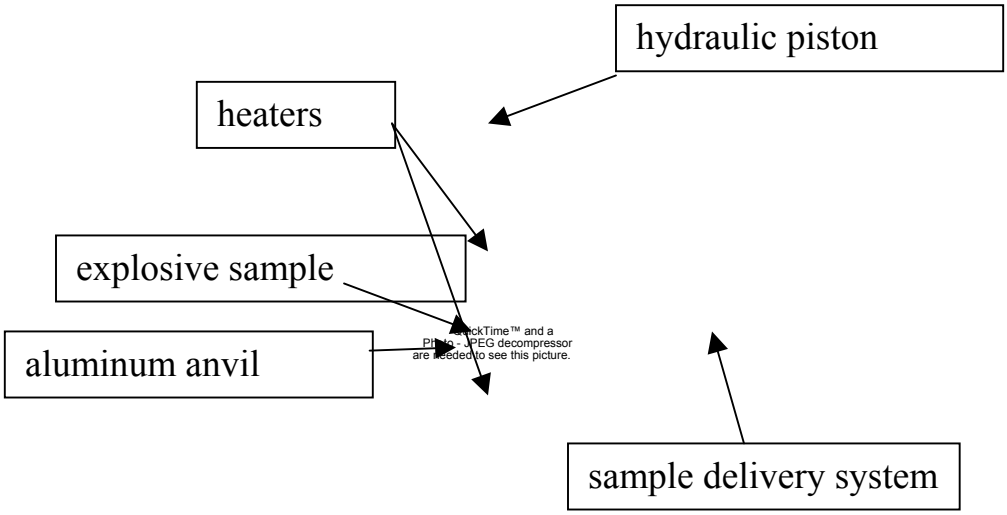
The thermal explosion experiments were conducted on two similarly designed ODTX apparatuses. The old unit was identical to the one described by Catalano et al. (1). The new system was designed to perform identical experiments but contained upgrades, modern equipment and new capabilities. A short description of the experiment and features of the new apparatus is presented below. Any similarity with the old unit will be noted. A picture of the new apparatus is shown in Figure 1.

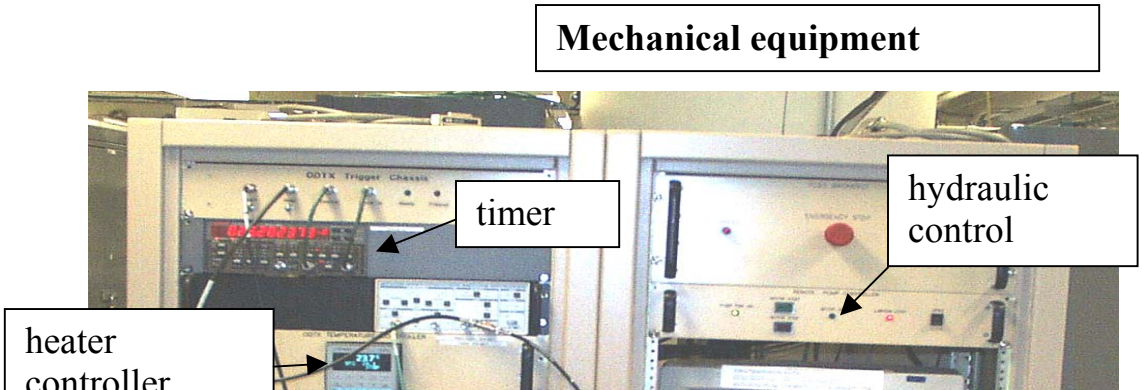
Anvils/sample holder - The anvil design is identical for both systems. The sample holder/confinement components consist of two identical cylindrical aluminum anvils (75-mm diameter x 50 mm long, 6061 T6 Al). Each anvil contains a 12.7 mm-diameter hemispherical cavity

and a 18.5 mm-diameter circular groove with a knife-edge bottom to accommodate a copper O-ring seal (3 mm-wide, Vacuum Products Corp., GK-075, P/N 191000). A circular copper ring clamped between the two knife-edges provides a gas-tight seal when two anvils are pressed together. The upper anvil is mounted to the piston surface of a hydraulic piston. The confinement pressure is calculated based on the cross-sectional area confined by the knife-edge. The anvil temperature is controlled by a calibrated resistive thermal devices (RTD) inserted into a 3 mm-diameter x 32 mm deep well at 3 mm below the anvil surface.

Hydraulic system – The new system uses a high throughput two-stage hydraulic pump (Power Team, Model D) for the opening and closing of the top anvil. A 16-ton double-acting hydraulic cylinder (RD-166, Enerpac) is used to move the top anvil (and the encased heater) and applies the closing (confinement) force. The bottom anvil, held in the heating block, is mounted rigidly. The standard operating hydraulic pressure is 20.5 MPa (giving a 150 MPa confinement pressure). This hydraulic

Figure 1. Picture of the One-Dimensional-Time-to-eXplosion System (ODTX)





pressure can be adjusted up to 35 MPa. A dynamic pressure gauge (Iomega, PX613) is mounted at the cylinder inlet to monitor the closing pressure as well as the relief pressure pulse immediately after the explosion.

Heating blocks - The heaters are brass cylindrical cups with encased heating elements (230V, 500-watt, Tempco Electric Co.) around the sidewall. The anvils fit tightly in the heaters. The heating is controlled *in-situ* through a temperature controller (OMEGA model CN300). The heater temperature is controlled by a resistive thermal device (RTD) located in the anvil. Typically, the RTDs are calibrated to within 0.3°C of a standard calibration probe.

Sample Delivery – The HE sample is delivered automatically by a pivoted mechanical jaw that grips the sample and then opens to release the sample when it is positioned above the sample cavity. The jaw is guided by a double-acting pneumatic piston (Tendra model 1) powered by 200 KPa compressed air. This new design is significantly faster than the swing-arm, vacuum suction/pressure release holder in the old unit. The new loading mechanism requires less than 1 second while the old system requires a total of about 10 seconds.

System control/data collection - The new system is fully automated and is interfaced with a computer. The operating software is LABVIEW. The control system consists of a Macintosh computer (Power PC 7600, Apple Co.) and interfaced temperature/pressure data collection modules (multimeters 2010, Keithley Instruments), temperature controller (CN3000, OMEGA Corp.), hydraulic pressure transducer (PX613, Omega Engineering) and pressure-data-processing oscilloscope (PCB 482R4, Hewlett-Packard Co.). The standard set-up has provision for 20 channels of input/output data, if additional diagnostics are used.

Time measurements - A digital timer (Model. 776, Keithley Instruments) records the time to explosion. The time is activated by a Reflective Optical Switch (Opto Switch No. R-280-A-W, Steven Engineering) mounted at the sample delivery arm. The explosive event is measured acoustically by a sensor embedded in the mounting assembly of the bottom anvil. Mechanical and optical position switches are located at various positions to monitor the locations of other moving parts.

Temperature measurements – Temperatures in the new system are measured with 4-wired RTDs (resistive thermal devices, 100 Ohm Platinum RTD with 3.2 mm-diameter ceramic end, P/N29229-T01, RdF Corporation). Most RTDs are accurate to within the manufacturer's suggested range of ± 0.3°C when calibrated against a known probe in our laboratory.

Sample preparation – The samples are 12.7 mm diameter spheres. Samples from previous work (2,3) were machined from pressed billets at 135 MPa and ambient temperature. They were pre-

coated with a thin layer (0.025 mm) of parylene N. Recent samples (from various sources) were pressed directly to shape in a die at 200 MPa under room temperature. Samples at various densities were made by varying the weight prior to pressing. Specimens at densities below about 1.20 g/cc contain loosely bounded particles that can flake off easily during handling.

Experiments involved materials from four separate TNT batches. Table 1 summarizes the four types of TNT and their characteristics. The first 3 batches (B-180, B-569 and C-175) were either military grade or from a commercial vendor. The recrystallized pure material was fine crystal that was crash-precipitated from a dissolved TNT/acetone solution. This material was first made in 1975.

EXPERIMENTAL RESULTS AND DISCUSSION

Initially, the temperature profile of the heated anvils was recorded to calibrate the heaters and verify the system operation. The new apparatus was then tested with TNT. A comparison of the operation of the two systems was done by investigating the thermal profile of the heated anvils and the time to explosion curves generated with the same materials.

Temperature measurements in old and new apparatuses - The anvil temperatures were measured differently in the two systems. In the old system, the temperature was recorded by a thermocouple (TC Type J, Omega Inc.) inserted in a 5 mm-thick disc sandwiched between the heated anvils. The tip of the TC was located about 19 mm from the center of the sample cavity. The temperature was recorded and this disc was manually removed before HE samples delivery. This transition took about 20 seconds before the heated anvils were reclosed. A small temperature reduction (about 1-2°C) was observed but was not corrected for in the measurement. This brief "cooling" period, however, is fairly consistent between tests, resulting in good reproducibility in the time to explosion measurements as observed over several years.

Table 1. Characteristics of historical and recent TNT samples

Variables/batch	**B-180**	**B-569**	**C-175**	**Recrystallized**
Source	MH VOL 7-654	MH VOL 7-654	HOLSTON C1B91 D003-040	Work ID. 75-166
ODTX date	1974	2000	2000	2000
Purity*	96 ± 2 %	94 ± 2.0 %	90 ± 3.4 %	100 ± 1%
Sample preparation	Pressed at 135 MPa & ambient temp. Machined to shape. Coated w/ 0.025 mm thick parylene-N	Pressed to shape at 200 MPa & ambient temp.	Pressed to shape at 200 MPa & ambient temp.	Pressed to shape at 200 MPa & ambient temp.

Sample weight, g	1.77	1.70	1.23 – 1.70	1.70
Sample density, g/cc	1.66	1.59	1.160-1.59	1.59

* Analysis for batch B-180 was done by Liquid Chromatography (previously unpublished data). Analysis for batches B-569, C-175 and recrystallized TNT was done by Liquid Chromatography/Mass Spectroscopy.

The reported temperature in the new ODTX unit is the average of two controlling RTDs inserted in the top and bottom anvils (one for each anvil). The controlling RTD is located in a well (3 mm–diameter x 32 mm deep) drilled into the side of the anvil, at 6.5 mm below its flat surface. Under well-controlled conditions, the calibrated controlling RTDs are found to be within 0.2 °C of the measured sample temperature (from another calibrated RTD placed at the center of the cavity). The fast sample delivery and anvil closure mechanisms in the new unit resulted in a significantly smaller heat loss (less than 0.5°C) during sample loading.

The difference in the reported temperatures for the old and new systems was quantified in a series in heating experiments, The disc used for the old apparatus was modified to accept a Cu ball (simulating the HE sample) fitted with a calibrated RTD in the center. This disc was placed in both systems and the temperatures were measured in the range between 200 and 300°C. Figure 2 compares the readings for the two systems. The TC readings, i.e., old ODTX temperatures, were consistently 2-4°C higher than that recorded from the calibrated RTD at the cavity center. We attribute this difference to systematic error, possibly from the uncalibrated TC or the meter or the TC placement or a combination of these factors. On the other hand, the controlled RTDs at the top and bottom anvils in the new unit were within 0.3°C of the Cu ball value. This difference could be reduced to less than 0.2°C by accounting for a slight offset between top and bottom anvil temperature due to their difference in thermal environment due to convective heat transfer to the top anvil (i.e., top anvil needed slightly less heat input). This is the limit of the new system temperature measurement accuracy. The temperature variance between the systems is consistent with an observed shift in the time-to-explosion recorded for the two apparatuses. We discuss this later in this paper.

Time measurement between the two apparatuses – The largest source of error in the time measurement in the old ODTX was attributed to the analog timer reading. It is precise to within 0.005 minute or about 0.3 seconds. The precision in the time measurement meter in the new ODTX is significantly higher (±1 μs). In repetitive time measurement tests in which timer was deliberately terminated by an electronic signal, the new system time measurement accuracy (reproducibility) is greater than 1 ms. Relative to other system errors, time measurement was not expected to significantly affect the variance in the explosion time.

Comparison of TNT decomposition with two ODTX units – Two series of TNT decomposition experiments were conducted to compare the relative performance of the two systems.

Identical conditions were maintained between the two sets of tests. The TNT samples (from batch C-175) were pressed at a density of 1.355 g/cc to account for volume increase due to melting and thermal expansion (see discussion in next section). The times to explosion on the two apparatuses are compared in Figure 3. The uncorrected data for the old system show slightly longer times when plotted with the results from the new system. We have determined earlier that the recorded thermocouple temperatures from the older unit ranges between 2°C and 3°C higher than those measured at the cavity center. If we corrected for this offset, the corrected time to explosion curves for the two systems show good reproducibility. Similar observations were also observed in ODTX experiments with another material (PBX-9501.) The results for both TNT and PBX-9501 (not discussed) provide adequate calibration for the new ODTX apparatus. We continue to conduct additional experiments to gain more working knowledge of the new system.

Thermal explosion of TNT at various densities – Because of large expansion of TNT upon melting, it was of interest to investigate this effect on the thermal decomposition kinetics. This can be studied simply by varying the density and hence mass of the pressed sample. Samples at varying masses can be conveniently pressed to a constant-volume (1.073 cm^3) spherical size for ODTX experiments. Sample density was varied by changing the pre-weight amount prior to pressing. Low-density materials such as those at 1.15 g/cc have visible pores and contained loosely packed particles.

We have found recently that tests with nominal densities (~1.6 g/cc) TNT samples produced large amount of smoke prior to explosion. Controlled heating experiments showed TNT flowing from between anvils, indicating leakage. This was likely due to the large volume expansion (~ 14%) associated with TNT melting at about 80°C (4). In addition, molten TNT would continue to expand at a rate equivalent to as much as 0.7% volume increase per 10°C (reference 5 for data between 85-120°C). An analysis of the heat flow in a 12.7 mm TNT sphere with a constant surface temperature was done using the solution provide by Carslaw and Jaeger (5). An isothermal condition (i.e., center temperature approaching 96% of surface temperature) in the solid sphere would be achieved after 179 s. This approximation is consistent with our experimental observations where explosion times in most tests were significantly longer than this value. It is interesting to note that the thermal decomposition behavior is remarkably reproducible even in the events that leaking was observed. This is consistent with rather reproducible kinetics observed by previous workers (in ref. 2,3) with full-density samples.

Experiments with TNT at lower densities (less than liquid TNT density) produced little smoking prior to explosive events in contrast to those at nominal densities where significant discharge of smoke was evident. For example, materials pressed at 1.355 g/cc (~ 82% TMD) were found to be mechanically robust for handling and produced well confined conditions during the

ODTX tests until thermal runaway. In addition, the faster new system showed no observable smoking prior to explosion event while the old system still showed occasional evident of leaking (i.e., smoking). We, however, can not directly correlate any effect between leakage and time to explosion.

The thermal explosion curves of TNT at a range of density between 1.15-1.60 g/cc are shown in Figure 4. Corrected data from the old unit and those from the new system were combined. The data were complicated by scatter in the measured times. While there appears to be a slight dependence on the times to explosion with sample density, the statistical significance of the results has not been analyzed. Experiments to investigate the new system reproducibility could be used to delineate the variances in the observed data, and are underway.

Effects of batch-to-batch variance – Four batches of TNT with various purity levels were included in this work to investigate the differences in the time to explosion that were noted in the early stage of this project. Recent results were from two available type-1 TNT flakes (B-569 and C-175). Historical data reported by previous workers (1, 2) were from a different batch of TNT (B-180). All

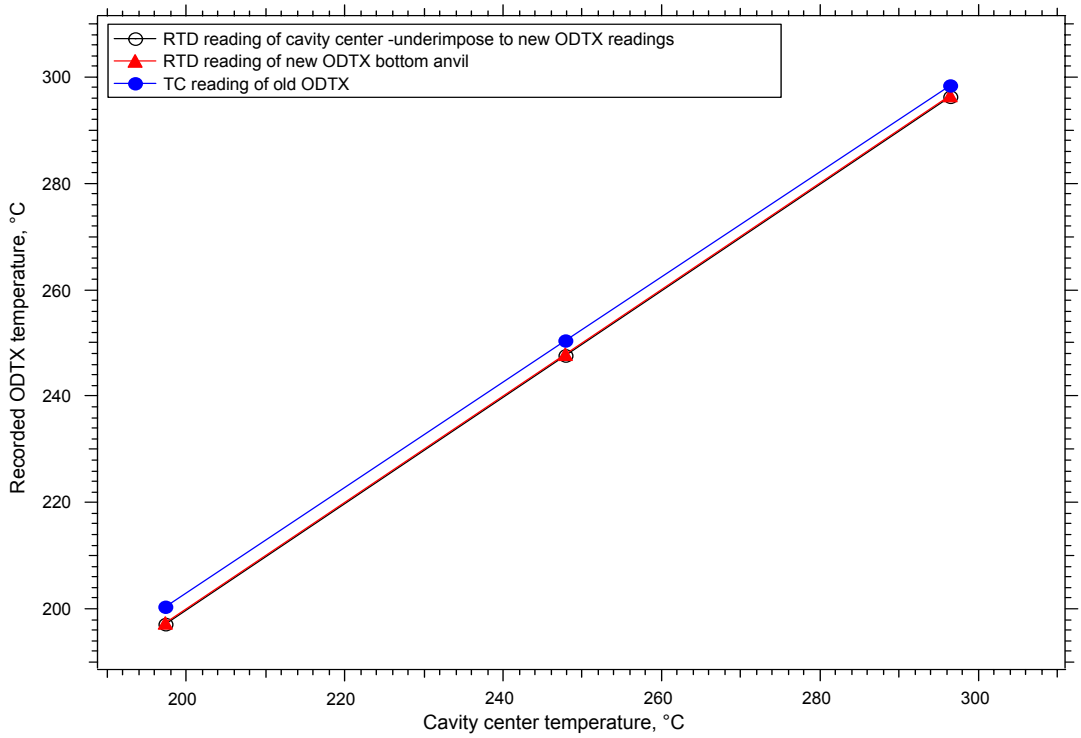


Figure 2. Comparison between temperature readings for the two systems. The values for the cavity center superimpose on those for new ODTX in this plot (within 0.2°C).

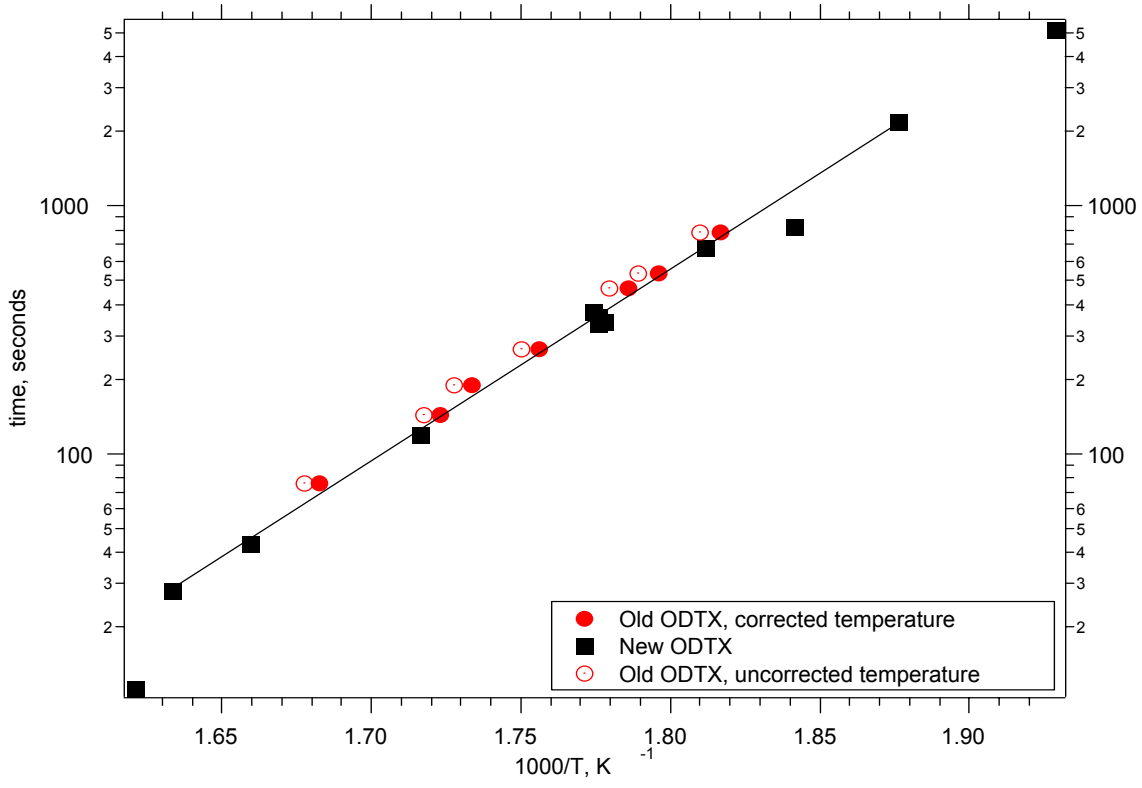


Figure 3 – Comparison of time to explosion for TNT (batch C-175) obtained with two ODTX apparatus. Thermocouple temperatures from the old ODTX were recorded 'as is' and corrected for offset between old and cavity temperature. RTD readings are from new system. TNT was pressed to 1.355 g/cc (~ 82% of solid TMD). Solid line is best-fit line of the new ODTX data in the range indicated to serve as a visual guide.

these experiments were conducted with the old ODTX unit. Recently, pure (recrystallized) TNT samples were studied with the new ODTX units. Characteristics and history of the four types of TNT are summarized in Table 1. The time to explosion of four batches of TNT versus anvil temperatures was presented in Figure 5. All temperature data were presented as is without correction for any temperature difference between the two systems because of uncertainty involved in the use of several thermocouples and RTDs over the course of many years. Temperature variance, however, is expected to be about 2°C.

In addition to the difference in apparatus and TNT sources, the samples were pressed and prepared in different procedures. The current samples (batch B569, C-175 and recrystallized materials) were pressed to 1.355 g/cc to accommodate a large expansion associated with TNT melting and subsequent liquid expansion prior to explosion. Samples from the earlier work (batch B-180, reference 1), on the other hand, had density around 1.66g/cc. Another variance noted from the historical TNT samples (from Ref. 2) is that the pressed parts (i.e., at 1.66 g/cc) were coated with 0.0254 mm thick Parylene N. While we do not understand the original purpose for this application, we speculate that this was used to retard the melting of TNT upon contact with the hot anvils. Our recent experience showed that the sample sizzled immediately after contacting the hot anvil. Some materials could be seen spilling out of the cavity prior to anvil closure. An insulating coat with Parylene N (melting point ~420°C, Parylene Technical data, Paratronix Inc.) could temporarily protect the sample before the anvils closure. Recent tests with samples (without coating) pressed at a lower density (i.e., less than liquid density) was found to emit much less smoke prior to anvil closure. Experiments with the new system, with a faster closing speed, gave a clean closure and produced no observable smoking prior to explosive events.

The large difference in the times to explosion is clearly attributed to sample purity associated with the batch-to-batch variances. While we did not study the effects of the parylene N coating, this thin and inert insulation layer is expected to produce a relatively small change to explosion time. Such an effect could be predicted with our model but this has not been determined.

The results suggest that impurity play a large role in the thermal decomposition chemistry of TNT. The pure recrystallized TNT shows the fastest time to explosion over the whole temperature region. The times to explosion appear to increase with impurity level associated with various batches. An increase of at least 10-fold is observed with increasing impurity from 0 to 10%. Additional analysis is underway to determine the composition and chemical nature of the impurities.

KINETIC MODELING OF TNT DECOMPOSITION USING CHEMICAL TOPAZ

Multi-step chemical kinetic decomposition modeling of TNT was first reported by Tarver et al. (2) and McGuire and Tarver (3). That TNT model was based on the ODTX data for Batch B-180, which is now known to contain approximately 4% impurities. These impurities are currently being analyzed, but most likely consist mainly of mono- and dinitrotoluenes that were not completely nitrated to trinitrotoluene during synthesis. The data (Fig. 5) show that the times to thermal explosion increase greatly with the percentage of impurities present from 100% recrystallized TNT to Batch B-180 (4%

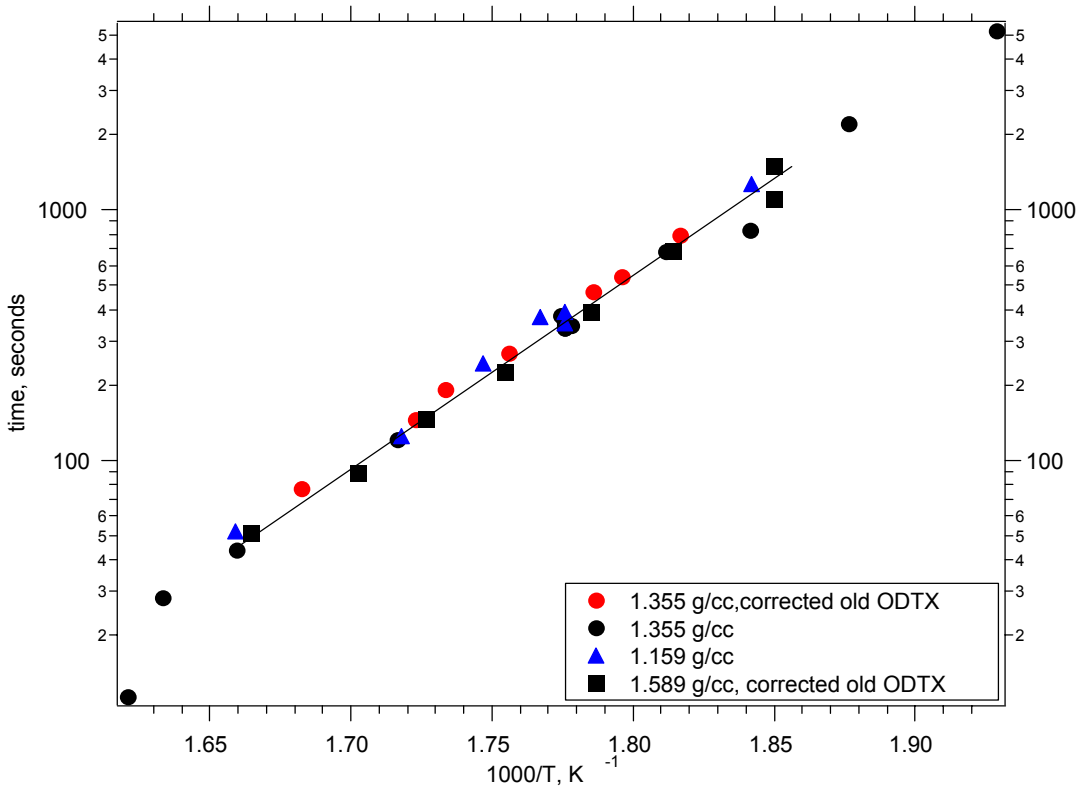


Figure 4. Effects of sample density on time to explosion. Densities were varied between 1.159 g/cc to 1.589 g/cc. Materials are from batch C-175. Solid line is best-fit line drawn through the linear region of the data at 1.589g/cc as visual guide.

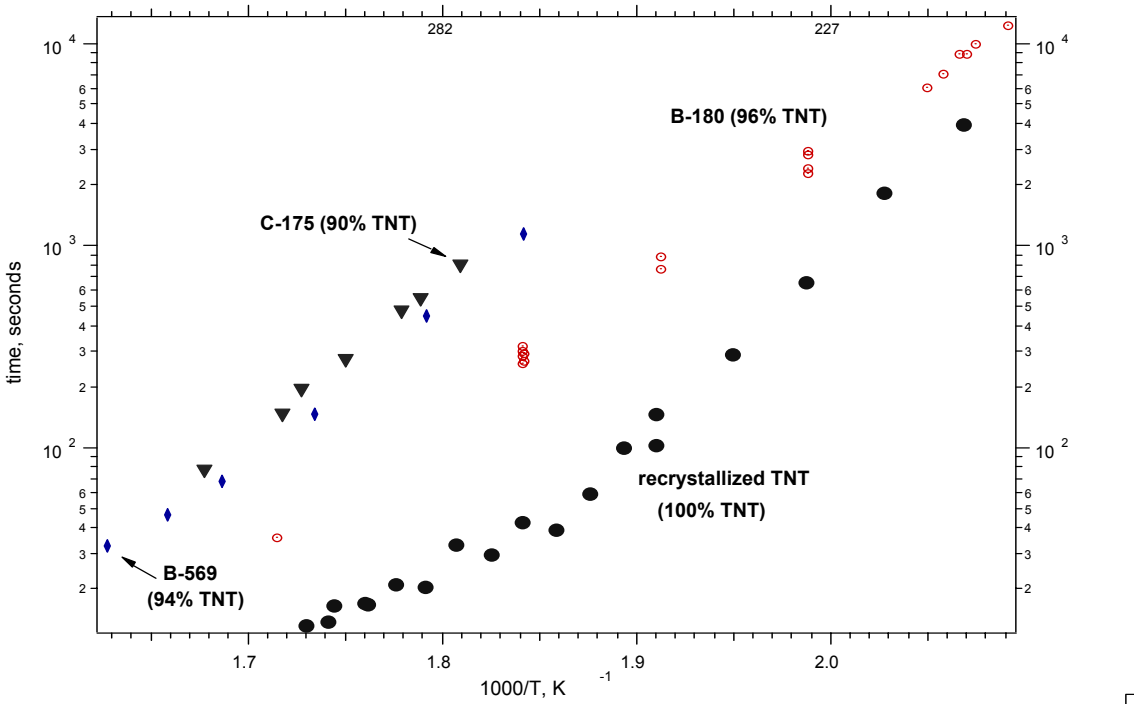


Figure 5. Effects of batch-to-batch variances on TNT decomposition kinetics. Recrystallized TNT was done on the new ODTX and other data were from the old ODTX. Temperature data were not corrected for a small offset between the two systems. See text for other details.

impurities) to Batches B-569 and C-175 (about 10% impurities). The previous decomposition model for TNT (2,3), which assumed an autocatalytic reaction based on very meager experimental kinetic information, was not adequate in simulating pure TNT decomposition.

We propose here a simple decomposition model for pure TNT that includes provisions to account for impurity decomposition. It also incorporates a Chemical TOPAZ code (7) that is a greatly improved version of the heat transfer codes used in the previous studies. Some differences are also expected due to improved numerical algorithms. The model consists of three chemical reactions to simulate the pure TNT ODTX data and an additional reaction to describe the effects of impurity. The four-species, three-reaction rate model for pure TNT uses the form:

$$\text{TNT} \rightarrow \text{Intermediate 1} \rightarrow \text{Intermediate 2} \rightarrow \text{Gaseous Products} \qquad \text{(A)}$$

which the reactions are:

$$A \rightarrow B \qquad (1)$$

$$B \rightarrow C \qquad (2)$$

$$C + C \rightarrow D \qquad (3)$$

where A is TNT, B is intermediate 1, C is intermediate 2 and D represents product gases. There are not sufficient experimental data to determine whether TNT exhibits any autocatalytic behavior. The heat of fusion of TNT, 93.3 J/g, is included in the heat transfer calculations at its melting point of 80.9˚C. The first two reactions in Equations (1) and (2) are endothermic since TNT has to break down into smaller, more reactive species before the exothermic processes can occur and cause thermal explosion (runaway reaction). Table 2 lists the thermal and chemical kinetics parameters used in the new model.

Figure 6 contains the comparison of the calculated times to explosion at various initial temperatures using the new TNT model with the ODTX results for pure recrystallized TNT. Also shown in Fig. 6 are the ODTX results for TNT with approximately 4% and 10% impurity levels. The differences in explosion times for these TNT batches are much greater than those measured for plastic bonded explosives (PBX) HE's containing various amounts of endothermic binders. For example, LX-10 (95% HMX and 5% Viton) and LX-04 (85% HMX and 15 % Viton) exhibit parallel

lines separated by only a small percentage of the total times to explosion in the ODTX apparatus (3). This is also true for TATB-based explosives, which have similar energies to TNT-based explosives (8). Therefore it is unlikely that the large time differences shown in Figs. 5 and 6 for the 90% TNT and 96% TNT batches are due to simple endothermic breakdown of non-reactive impurities. It appears likely that these impurities react with the intermediate products of TNT decomposition before the exothermic reactions

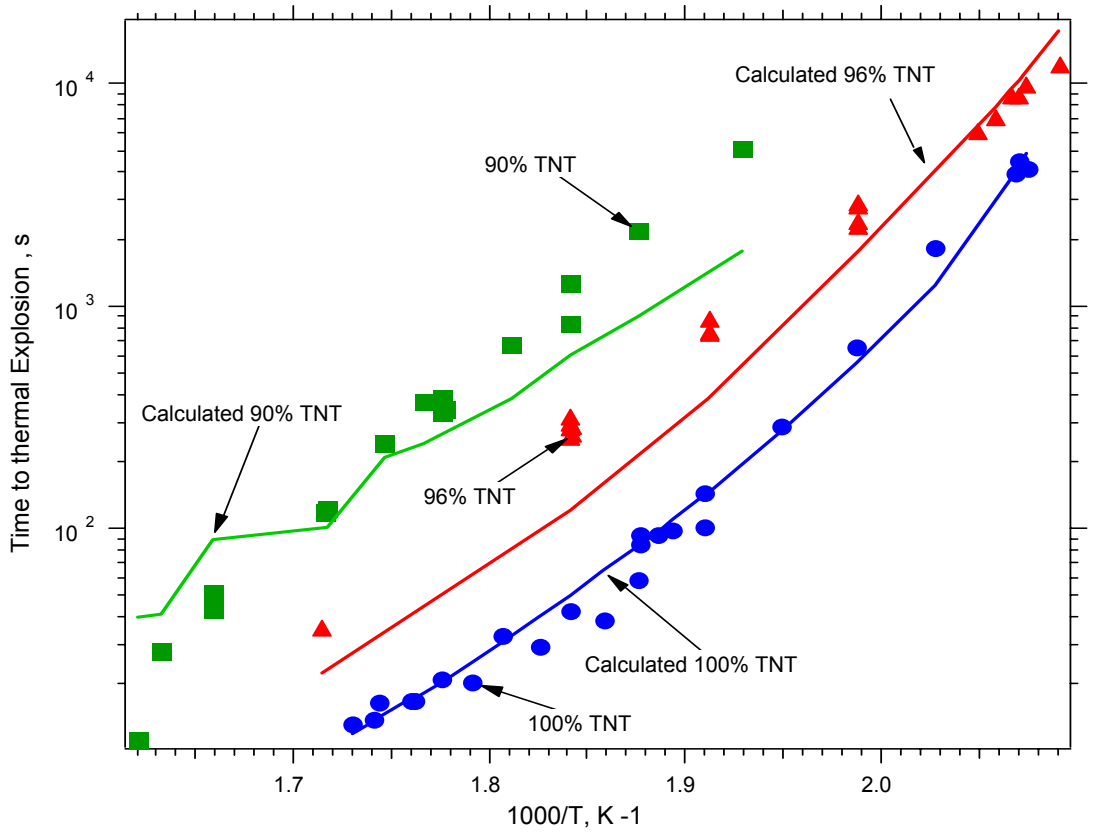


Figure 6. Comparison of experimental data and modeling results for various TNT samples. Kinetics model is based on 5-species,4-reaction with parameters given in Table 2. Pure TNT decomposition doesn't activate reaction 4.

Table 2. Thermal and Kinetic Parameters used in the TNT decomposition model

Properties	TNT	Reaction 1	Reaction 2	Reaction 3	Reaction 4
Heat of fusion, J/g	99.3				
Melting point, °C	80.9				
Thermal conductivity, J/cm s °C	2.59×10^{-3}				
Heat capacity J/g°C	1.1297				
Heat of reaction, J/g		209.2	209.2	- 3765	8368
Ln Z		57	52.8	37.5	40
Activation energy, 1/K		32500	30000	22142	20000
Reaction order		1	1	2	3 for Intermediate 2

					1 for Impurity

can occur and thus delay the onset of thermal explosion until the impurities are decomposed. Figure 6 contains calculated curves for 96% TNT and 90% TNT assuming the reaction

$$\text{Intermediate 2} + \text{Impurity} \rightarrow \text{Impurity Products} \qquad (4)$$

occurs before the third (exothermic) reaction in Eq. (3) can proceed. Table 2 also lists the parameters used for this reaction, which assumed that three moles of Intermediate 2 react with each impurity mole in a highly endothermic process. These calculations underestimate most of the measured increases in time to explosion, especially for the 90% TNT batches, and are included as a first approximate description of the complex chemistry that is occurring. More detailed chemical kinetic modeling can be developed when additional data on the nature of the impurities and their effects on TNT decomposition rates are obtained.

ACKNOWLEDGMENT

We gratefully acknowledge Greg Sykora, Kent Montgomery, Dan Greenwood and Barry Levine for their assistance in the development of the new system. We thank Jerry Dow for providing funding. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

REFERENCES

1. E. Catalano, R. McGuire, E. L. Lee, E. Wrenn, D. Ornellas, and J. Walton, *Sixth International Symposium on Detonation Proceedings,* p. 214, Office of Naval Research, ACR-221, Coronado, CA (1976).
2. C. M. Tarver, R. R. McGuire, E. L. Lee, E. W. Wrenn, and K. R. Brein, *Seventeenth Symposium (International) on Combustion*, Leeds, UK, p. 1407 (1978).
3. R. R. McGuire and C. M. Tarver, *Seventh International Symposium on Detonation*, Naval Surface Weapons Center, Annapolis, MD, p. 56 (1981).
4. W. A. Gey et al. *J. Amer. Chem. Soc*., **78**, 1803 (1956).

5. H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids*, Second Edition, Oxford University Press, p. 233 (1959).
6. H. H. Cady and W. H. Rogers, Report LA-2696, US Atomic Energy Commision (1962).
7. A. L. Nichols III and K. W. Westerberg, Numerical Heat Transfer, Part B, **23**, 489 (1993).
8. S. K. Chidester, C. M. Tarver, L. G. Green, and P. A. Urtiew, *Combustion and Flame* **110**, 264 (1997).